Constrained Least Squares Linear Spectral Unmixture by the Hybrid Steepest Descent Method

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1 Introduction

A closed polyhedron is the intersection of finite number of closed half spaces, i.e., the set of points satisfying finite number of linear inequalities, and is widely used as a constraint in various application, for example specifications or constraints in signal processing or estimation problems, resource restrictions in financial applications and feasible sets of probability distributions. By the progress of the convex analysis and the fixed point theory of nonexpansive mapping, a number of convex projection based algorithms are proposed (for example, Bauschke et al, 1997; Combettes, 1993; Yamada et al, 1998–2002). In this paper, to apply efficiently such methods to problems with polyhedral constraints, we propose a simple solution to the problem of the best approximation to the certain polyhedron. By applying this solution to the the hybrid steepest descent method (Ogura et al, 2002; Yamada et al 1998; Yamada 2001), we also present two algorithms for a linear spectral unmixing problem. The proposed method enable us to deal with constraints and variety of cost function (for example, least square residual, Kullback-Leibler Divergence) as well as various a priori knowledge with great flexibility.

The rest of this paper is organized as follows. The next section contains brief preliminaries on a linear unmixing problem and the hybdid steepest descent method. In the third section, we present a simple solution to the best approximation problem. In the last section, we show the algorithmic solution to the inversion of image spectrometry data by using projection based convexly constrained pseudoinverse algorithm.

2 Preliminaries

A. Best Approximation Problem to Polyhedron

Let \mathcal{H} be a real Hilbert space with inner product $\langle \cdot, \cdot \rangle$ and norm $\| \cdot \|$. Suppose that N_1 hyperplains and N_2 closed half spaces are given by $S_{1,i} := \{u \in \mathcal{H} \mid \langle \rho_{1,i}, u \rangle = c_{1,i} \}$ and $S_{2,j} := \{u \in \mathcal{H} \mid \langle \rho_{2,j}, u \rangle \geq c_{2,j} \}$ respectively, where $\rho_{1,i} \in \mathcal{H}$, $c_{1,i} \in \mathbb{R}$, $\rho_{2,j} \in \mathcal{H}$ and $c_{2,j} \in \mathbb{R}$ $(i = 1, \dots, N_1, j = 1, \dots, N_1)$. Then, the problem of our interests is

Minimize
$$||u - u_0||$$
 over $S := \left(\bigcap_{i=1}^{N_1} S_{1,i}\right) \cap \left(\bigcap_{j=1}^{N_2} S_{2,j}\right) \neq \emptyset$ (1)

for given $u_0 \in \mathcal{H}$. It is known that the problem (1) has unique minimizer. (This fact holds for general nonempty closed convex set $C(\subset \mathcal{H})$ instead of the polyhedron S. In this case the minimizer is denoted by $P_C(u_0)$.) An algorithm found in (Wolfe, 1976) gives the solution of (1) if all vertex is known. Some algorithms based on the cycric projection or the parallel projection methods (Bauscheke 1997; Combettes, 1993; Stark, 1998; Yamada 2001; Yamada et al, 1998) can be applicable to compute such a projection (which are computationally easy but require infinitely many iterations in general). The quadratic

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programming techniques can also be available, for example general active-set methods (Gill et al, 1978; Goldfarb et al, 1983) (which are finitely convergent but somewhat complicated in handling active-sets selection). Although, the method proposed in this paper can be essentially interpreted as an active-set method, we show in Section 3 that the complete determination of the active set is possible if the polyhedron satisfies condition (2). For example, the condition is fullfilled if

$$N_1 = 0$$
 and $\langle \rho_{2,i}, \rho_{2,i} \rangle \leq 0$ for all $i \neq j$,

(see Section 3 for other examples.) Based on this fact, we propose a simple algorithmic solution to the problem (1), which requires at most only $N_1 + N_2$ times iterations to obtain the solution.

B. Hybrid Steepest Descent Method

A fixed point of a mapping $T: \mathcal{H} \to \mathcal{H}$ is a point $u \in \mathcal{H}$ such that T(u) = u. $Fix(T) := \{u \in \mathcal{H} \mid T(u) = u\}$ denotes the set of all fixed points of T. A mapping $T: \mathcal{H} \to \mathcal{H}$ is called κ -Lipschitzian (or κ -Lipschitz continuous) over $S \subset \mathcal{H}$ if there exists $\kappa > 0$ such that $||T(u) - T(v)|| \le \kappa ||u - v||$ for all $u, v \in S$. In particular, a mapping $T: \mathcal{H} \to \mathcal{H}$ is called (i) nonexpansive if $||T(u) - T(v)|| \le ||u - v||$ for all $u, v \in \mathcal{H}$; (ii) attracting nonexpansive if $T: \mathcal{H} \to \mathcal{H}$ is a nonexpansive mapping satisfying ||T(u) - f|| < ||u - f|| for all $f \in Fix(T) \neq \emptyset$ and $u \notin Fix(T)$. The convex projection P_C onto a nonempty closed convex set C is attracting nonexpansive. A mapping $\mathcal{F}: \mathcal{H} \to \mathcal{H}$ is called monotone over $S \subset \mathcal{H}$ if $\langle \mathcal{F}(u) - \mathcal{F}(v), u - v \rangle \geq 0$ for all $u, v \in S$. Indeed, a mapping \mathcal{F} which is monotone over $S \subset \mathcal{H}$ is called η -strongly monotone or just strongly monotone over $S \subset \mathcal{H}$ is called η -strongly monotone or just strongly monotone over $S \subset \mathcal{H}$ is called η -strongly monotone or just strongly monotone over $S \subset \mathcal{H}$ is called $S \subset \mathcal{H}$ is called

The following fact is an algorithmic solution to convex constrained pseudoinverse based on the hybrid steepst descent method (Yamada et al 1998; Yamada 2001).

Fact 1 (Yamada, 1999, 2001) Suppose that $\mathcal{C} := \arg\inf_{x \in K} \|Ax - b\|_{(m)} \neq \emptyset$ for a given bounded linear mapping $A : \mathcal{H} \to \mathbb{R}^m$, a possibly perturbed vector $b = (b_1, \dots, b_m)^T$ and a nonempty bounded closed convex set $K \subset \mathcal{H}$. Suppose $a_i \in \mathcal{H}$ $(i = 1, \dots, m)$ are determined to follow $Ax = (\langle a_1, x \rangle, \dots, \langle a_m, x \rangle)$. Let $T(x) := P_K \sum_{i=1}^m \frac{\|a_i\|^2}{\sum_{j=1}^m \|a_j\|^2} \left(x - \frac{\langle a_i, x \rangle - b_i}{\|a_i\|^2} a_i\right)$. Suppose that $\Theta : \mathcal{H} \to \mathbb{R}$ is convex over K and Gâteaux differentiable with derivative Θ' κ -Lipschitzian and η -strongly monotone over K. Then, the sequence $(u_n)_{n \geq 0} \subset \mathcal{H}$, generated by $u_{n+1} = T(u_n) - \frac{1}{n+1}\Theta'(T(u_n))$ with arbitrary u_0 , converges to uniquely existing minimizer of Θ over K.

Remark 1 If K is bounded, $\mathcal{C} \neq \emptyset$ is ensured (Yamada et al, 1998).

The following is a variation of the hybrid steepst descent method, which plays important role to give a flexible linear unmixing algorithm in Section 4.

Fact 2 (Ogura et al, 2002a, 2002b) Assume that \mathcal{H} is finite dimensional real Hilbert space. Suppose that $T: \mathcal{H} \to \mathcal{H}$ is an attracting nonexpansive mapping with bounded Fix(T). Let a function $\Theta: \mathcal{H} \to \mathbb{R}$ be convex and Gâteaux derivative over $T(\mathcal{H})$ with derivative Θ' κ -Lipschitzian. Then, the sequence $(u_n)_{n\geq 0} \subset \mathcal{H}$, generated by $u_{n+1} := T(u_n) - \frac{1}{n+1}\Theta'(T(u_n))$ with arbitrary u_0 satisfies $\lim_{n\to\infty} d(u_n, \arg\inf_{x\in Fix(T)}\Theta(x)) = 0$ $(d(u,C):=\inf_{v\in C}\|u-v\|$ denotes the distance from $u\in\mathcal{H}$ onto a nonempty closed convex set C).

3 Main Results

Define a closed polyhedron S as in (1) Under the assumption that $\rho_{2,i}^{(1,N_1)}$'s, defined by (3), satisfy

$$\langle \rho_{2,i}^{(1,N_1)}, \rho_{2,j}^{(1,N_1)} \rangle \le 0 \text{ for all } i \ne j,$$
 (2)

the following algorithm enable us to compute $P_S(u_0)$ for arbitraty $u_0 \in \mathcal{H}$ if $S \neq \emptyset$, as well as to verify S is empty or not.

Algorithm 1: Let $\rho_{1,i}^{(1,0)} := \rho_{1,i}$, $c_{1,i}^{(1,0)} := c_{1,i}$, $\rho_{2,i}^{(1,0)} := \rho_{2,i}$, $c_{2,i}^{(1,0)} := c_{2,i}$ and $u^{(1,0)} := u_0$. For simplicity, define a function $\theta : \mathcal{H} \times \mathcal{H} \times \mathbb{R} \to \mathbb{R}$ as

$$\theta(u, v, w) := \begin{cases} \frac{\langle u, v \rangle - w}{\|u\|^2} & (u \neq 0) \\ 0 & (\text{otherwise}). \end{cases}$$

Define the sequences $(\rho_{1,j}^{(1,i)})_{0 \leq i \leq N_1}$, $(c_{1,j}^{(1,i)})_{0 \leq i \leq N_1}$, $(\rho_{2,j}^{(1,i)})_{0 \leq i \leq N_1}$ and $(c_{2,j}^{(1,i)})_{0 \leq i \leq N_1}$ as follows:

$$\rho_{1,j}^{(1,i+1)} := \rho_{1,j}^{(1,i)} - \theta(\rho_{1,i+1}^{(1,i)}, \rho_{1,j}^{(1,i)}, 0) \rho_{1,i+1}^{(1,i)}
c_{1,j}^{(1,i+1)} := c_{1,j}^{(1,i)} - \theta(\rho_{1,i+1}^{(1,i)}, \rho_{1,j}^{(1,i)}, 0) c_{1,i+1}^{(1,i)}
\rho_{2,j}^{(1,i+1)} := \rho_{2,j}^{(1,i)} - \theta(\rho_{1,i+1}^{(1,i)}, \rho_{2,j}^{(1,i)}, 0) \rho_{1,i+1}^{(1,i)}
c_{2,j}^{(1,i+1)} := c_{2,j}^{(1,i)} - \theta(\rho_{1,i+1}^{(1,i)}, \rho_{2,j}^{(1,i)}, 0) c_{1,i+1}^{(1,i)}.$$
(3)

If there exists i such that $c_{1,i}^{(1,N_1)} \neq 0$, then $S = \emptyset$ and this algorithm completes. Otherwise, define $(u^{(1,i)})_{0 \geq i \geq N_1}$ by

$$u^{(1,i+1)} := u^{(1,i)} - \theta(\rho_{1,i+1}^{(1,i)}, u^{(1,i)}, c_{1,i+1}^{(1,i)}) \rho_{1,i+1}^{(1,i)}.$$

and let $\rho_{2,i}^{(2,0)} := \rho_{2,i}^{(1,n)}, \ c_{2,i}^{(2,0)} := c_{2,i}^{(1,n)}$ and $u^{(2,0)} := u^{(1,N_1)}$. While it hold for some i that $\rho_{2,i}^{(2,n)} \neq 0$ and $\langle \rho_{2,i}^{(2,n)}, u_n \rangle < c_{2,i}$, repeat from n=0 that

$$\rho_{2,j}^{(2,n+1)} := \rho_{2,j}^{(2,n)} - \theta(\rho_{2,i}^{(2,n)}, \rho_{2,j}^{(2,n)}, 0) \rho_{2,i}^{(2,n)}
c_{2,j}^{(2,n+1)} := c_{2,j}^{(2,n)} - \theta(\rho_{2,i}^{(2,n)}, \rho_{2,j}^{(2,n)}, 0) c_{2,i}^{(2,n)}
u^{(2,n+1)} := u^{(2,n)} - \theta(\rho_{2,i}^{(2,n)}, \rho_{2,j}^{(2,n)}, c_{2,i}^{(2,n)}) \rho_{2,i}^{(2,n)}.$$
(4)

If there exists i such that $\rho_{2,i}^{(2,N_3)}=0$ and $c_{2,i}^{(2,N_3)}>0$ when this iteration stops at $n=:N_3$, then $S=\emptyset$, otherwise $u^{(2,N_3)}$ is $P_S(u_0)$.

By the following lemma, it is easily verified that (a) the iterative step of (4) surely stops at some $n(=N_3) \leq N_2$; (b) if there exists i such that $c_{1,i}^{(1,N_1)} \neq 0$, then $S = \emptyset$; (c) if $c_{1,i}^{(1,N_1)} = 0$ for all $1 \leq i \leq N_1$ and there exists j such that $\rho_{2,j}^{(2,n)} = 0$ and $c_{2,j}^{(2,n)} < 0$, then $S = \emptyset$; (d) if $c_{1,i}^{(1,N_1)} = 0$ for all $1 \leq i \leq N_1$ and $\rho_{2,j}^{(2,n)} \geq c_{2,j}^{(n)}$ for all $1 \leq j \leq N_2$, then $u^{2,n} = P_S(u_0)$.

Lemma 1 Suppose that $\rho_{2,i}^{(1,N_1)}$ satisfies (2). Let $S_{i,j}^{(k,l)} := \{u \in \mathcal{H} \mid \langle \rho_{i,j}^{(k,l)}, u \rangle \geq c_{i,j}^{(k,l)} \}$, $S^{(1,i)} := (\bigcap_{j=1}^{N_1} S_{1,j}^{(1,i)}) \cap (\bigcap_{j=1}^{N_2} S_{2,j}^{(1,i)})$ and $S^{(2,i)} := \bigcap_{j=1}^{N_2} S_{2,j}^{(2,i)}$. Then:

$$(a) \ \langle \rho_{2,i}^{(2,n)}, \rho_{2,j}^{(2,n)} \rangle \leq 0 \ \text{for all} \ i \neq j \Rightarrow \langle \rho_{2,i}^{(2,n+1)}, \rho_{2,j}^{(2,n+1)} \rangle \leq 0 \ \text{for all} \ i \neq j,$$

(b)
$$|\{i \in \{1, \dots, N_2\} \mid \rho_{2,i}^{(2,n+1)} = 0\}| \le |\{i \in \{1, \dots, N_2\} \mid \rho_{2,i}^{(2,n)} = 0\}| - 1,$$

(c)
$$S^{(i,j)} = \emptyset \Leftrightarrow S^{(i,j+1)} = \emptyset$$
,

(d) If
$$c_{1,i}^{(1,N_1)} = 0$$
 for all i, then $S^{(2,0)} = \emptyset \Leftrightarrow S^{(1,N_1)} = \emptyset$,

(e)
$$S^{(i,j)} \neq \emptyset \Rightarrow P_{S^{(i,j+1)}}(u^{(i,j+1)}) = P_{S^{(i,j)}}(u^{(i,j)})$$

(f) If
$$c_{1,i}^{(1,N_1)} = 0$$
 for all i , then $S^{(1,N_1)} \neq \emptyset \Rightarrow P_{S^{(2,0)}}(u^{(2,0)}) = P_{S^{(1,N_1)}}(u^{(1,N_1)})$.

(The proof of this lemma is omitted.)

Note: The following is an example of polyhedron satisfying (2):

$$\left\{ u = (x_1, \dots, x_m) \in \mathbb{R}^m \mid x_i \ge 0 \text{ for all } i \text{ and } \sum_{i=1}^m w_i x_i = 1 \right\}$$

where $w_i > 0$ $(i = 1, \dots, m)$. If $w_i = 1$ for all $i = 1, \dots, m$, this polyhedron represents the feasible set of probability distribution. The following is another example:

$$\left\{ u = (x_1, \dots, x_m) \in \mathbb{R}^m \mid x_i \ge 0 \text{ for all } i \text{ and } \sum_{i=1}^m w_i x_i \le 1 \right\}$$

where $w_i > 0$ $(i = 1, \dots, m)$. All closed affine spaces are also examples satisfying (2).

4 Application to the Linear Unmixing for Imaging Spectrometry

In this section, we apply the Algorithm 1 in the previous section to the problem of an inversion of image spectrometry data. In the imaging spectrometry, a pixel is generally mixed by a number of materials present in the scene as follows (Chang et al, 2000; Clark et al, 1998; Heinz et al, 2001; Settle, 1993, 1996; Shimabukuro et al, 1991):

$$r = M\alpha + e, (5)$$

where $r=(r_1,\cdots,r_l)^T\in\mathbb{R}^l$ is an observed image pixel, $M\in\mathbb{R}^{l\times p}$ is a material signature, $\alpha=(\alpha_1,\cdots,\alpha_p)^T\in\mathbb{R}^p$ is an abundance vector, e is a noise or a measurement error, l is the number of spectral bands and p is the number of reference materials. Each r_i represents observed reflectance of each band, and each α_i represents abundance fraction associated with i-th material and α_i 's satisfy $\sum_{i=1}^p \alpha_i = 1$ and $\alpha_i \geq 0$ for all $i=\{1,\cdots,p\}$, each component $m_{i,j}$ of signature matrix M is represents the reference reflectance of i-th band of the j-th material reference spectral signature.

Then, a linear unmixing method attempts to estimate the unknown abundance vector α from the observed image pixel r. Such an inversion process of the linear mixture model is required to achieve the tasks of material discrimination, detection, classification, quantification, etc.

The estimation problem is the following polyhedron constrained inverse problem:

Minimize
$$||r - M\alpha||_{(l)}$$

subject to $\alpha \in S$ (6)

where $S := \{ \alpha \in \mathbb{R}^p \mid \alpha_i \geq 0 \text{ for all } i = \{1, \dots, p\} \text{ and } \sum_{i=1}^p \alpha_i = 1\}, \text{ and } \| \cdot \|_{(l)} \text{ denotes the standard norm defined in Euclid space } \mathbb{R}^l.$

The quadratic programming based methods are developed in (Settle, 1993; Shimabukuro et al, 1991) to solve (6). To avoid the computational complexity of these method, an penalty function based method is employed in (Heinz et al, 2001; Chang et al, 2000). These methods assume that the matrix M has full rank. Unfortunately this assumption does not hold in some practical situations because there are so many reference signatures and sometimes signature vectors may automatically generated from observed image (Chang et al, 2000; Ren et al, 2000).

Algorithm 2: By letting $a_i := m_{i,*}$, $(m_{i,*}$ denote *i*-th row-vector) and K := S, Fact 1 realize the algorithm to Minimize a function $\Theta(u)$ over the solution of (6).

Remark 2 This algorithm does not require for M to be full rank. In addition, unlike conventional techniques, Algorithm 2 can impose additional criteria Θ to the problem (6). Indeed, if M does not have full rank, the solution of (6) may not be unique. For such a case, Fact 1 can find unique minimizer of Θ over the set of all solution of (6). We can take Θ as energy function or other function reflecting some spatial information.

Algorithm 3: By letting $\Theta(\alpha) := ||r - M\alpha||_{(l)}$, Fact 2 realize the algorithm to Minimize $||r - M\alpha||_{(l)}$ over Fix(T).

Note: We can find a solution of (6) by using attracting nonexpansive mapping $T := P_S$ because $Fix(P_S) = S$.

Remark 3 Unlike conventional techniques, Algorithm 3 can deal with more flexible constraint than that of (6) by substituting T. By using $T:=P_S\sum_{i=1}^N w_i P_{C_i}$, we can find a point $u\in \arg\inf_{x\in K_\Phi}\|r-M\alpha\|_{(l)}$ where C_i is nonempty closed bounded set and $w_i\in (0,1]$ and $K_\Phi:=\arg\inf_{x\in S}\sum_{i=1}^N w_i d^2(x,C_i)$. This T enable us to handle additional a priori knowledges reflected by $C_i's$, which is expected to be obtained from spatial or statistical information in the hyperspectral imaging. See (Yamada, 2001) for the properties of K_Φ and other example of attracting nonexpansive mapping T. Fact 2 can also take other Θ for residual minimization, which means Fact 2 potentially has capability to use various distances, which is more suitable for the hyperspectral imaging, for instance, Kullback-Leibler Divergence $\Theta(\alpha):=\sum_{i=1}^l \langle m_{i,*},\alpha\rangle\log\frac{\langle m_{i,*},\alpha\rangle}{r_i}$ or Spectral Information Divergence (Chang, 2000) $\Theta(\alpha):=\sum_{i=1}^l \langle m_{i,*},\alpha\rangle\log\frac{\langle m_{i,*},\alpha\rangle}{r_i}+\sum_{i=1}^l r_i\log\frac{r_i}{\langle m_{i,*},\alpha\rangle}$.

Numerical Experiment 1

We choose 3 independent reference spectral signature vector from USGS Digital Spectral Library: splib(vers.4) for AVIRIS. $m_{*,1}$ is record No.120 Copiapite, $m_{*,2}$ is record No.231 Jarosite, $m_{*,3}$ record No.171 Gaothite ($m_{*,j}$ denote j-th column-vector of the matrix M). These signature has band number l=224. Figure 1 shows the reference spectral signature vectors $m_{*,1}$, $m_{*,2}$ and $m_{*,3}$.

Abundance of each material are set to Copiapite 60%, Jarosite 30%, Gaothite 10%, thus abundance vector is $\alpha = (0.6, 0.3, 0.1)^T$.

Sample observation data r are randomly generated by (5) with 30:1 SNR gaussian error e.

Then, inversion was made by (a) the algorithm of Fact 1 (with $\Theta(u) := ||u||$) and (b) the algorithm of Fact 2 (with $T := P_S$) and (c) FCLS algorithm ($\delta = 10^{-5}$) proposed in (Chang et al, 2000; Heinz et al, 2001). The simulation results of 3 data are shown in Table 1.

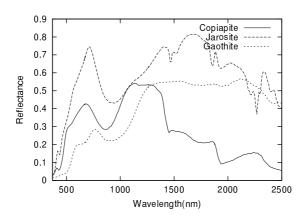


Figure 1: The reference spectral signatures.

	estimated abundance α	$ r - MP_S(\alpha) _{(l)}^2$
(a), Data No.1	(0.603551, 0.305009, 0.091440)	$1.853264252604 \times 10^{-2}$
(b), Data No.1	(0.603404, 0.305436, 0.091159)	$1.853141617604 \times 10^{-2}$
(c), Data No.1	(0.603405, 0.305436, 0.091160)	$1.853141617794 \times 10^{-2}$
(a), Data No.2	(0.606399, 0.304080, 0.089520)	$2.044290704859 \times 10^{-2}$
(b), Data No.2	(0.605570, 0.304144, 0.090286)	$2.043725005123 \times 10^{-2}$
(c), Data No.2	(0.605570, 0.304144, 0.090286)	$2.043725005186 \times 10^{-2}$
(a), Data No.3	(0.596860, 0.302069, 0.101070)	$1.604000824838 \times 10^{-2}$
(b), Data No.3	(0.597202, 0.301896, 0.100902)	$1.603884893825 \times 10^{-2}$
(c), Data No.3	(0.597202, 0.301897, 0.100902)	$1.603884893852 \times 10^{-2}$

Table 1: Result of Experiment 1.

	estimated abundance α	$ r - MP_S(\alpha) _{(l)}^2$
(d), Data No.1	(0.451246, 0.198576, 0.350178)	$1.902200569304 \times 10^{-2}$
(e), Data No.1	(0.638525, 0.326029, 0.035446)	$1.898692271721 \times 10^{-2}$
(d), Data No.2	(0.453241, 0.196296, 0.350463)	$2.101749344546 \times 10^{-2}$
(e), Data No.2	(0.640458, 0.324286, 0.035257)	$2.096505360051 \times 10^{-2}$
(d), Data No.3	(0.447391, 0.202981, 0.349627)	$1.622697188668 \times 10^{-2}$
(e), Data No.3	(0.636149, 0.328172, 0.035679)	$1.622479447754 \times 10^{-2}$

Table 2: Result of Experiment 2.

Numerical Experiment 2

To examine the case that signature vectors are dependent, replace $m_{*,3}$ by $0.6m_{*,1}+0.4m_{*,1}$ and make same experiment with (d) the algorithm of Fact 1 and (e) the algorithm of Fact 2. The simulation results of 3 data are shown in Table 2.

The results of Experiments 1 and 2 show that the proposed methods gives almost same accuracy as that given by conventional method although the proposed methods only requires loose assumptions and has flexibility to optimality criteria and constraints.

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